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the Analytical Scientist

Is Analytical Science Sexist?

Six (female) chemists tackle equality, glass ceilings – and the prospect of an all-women Power List.

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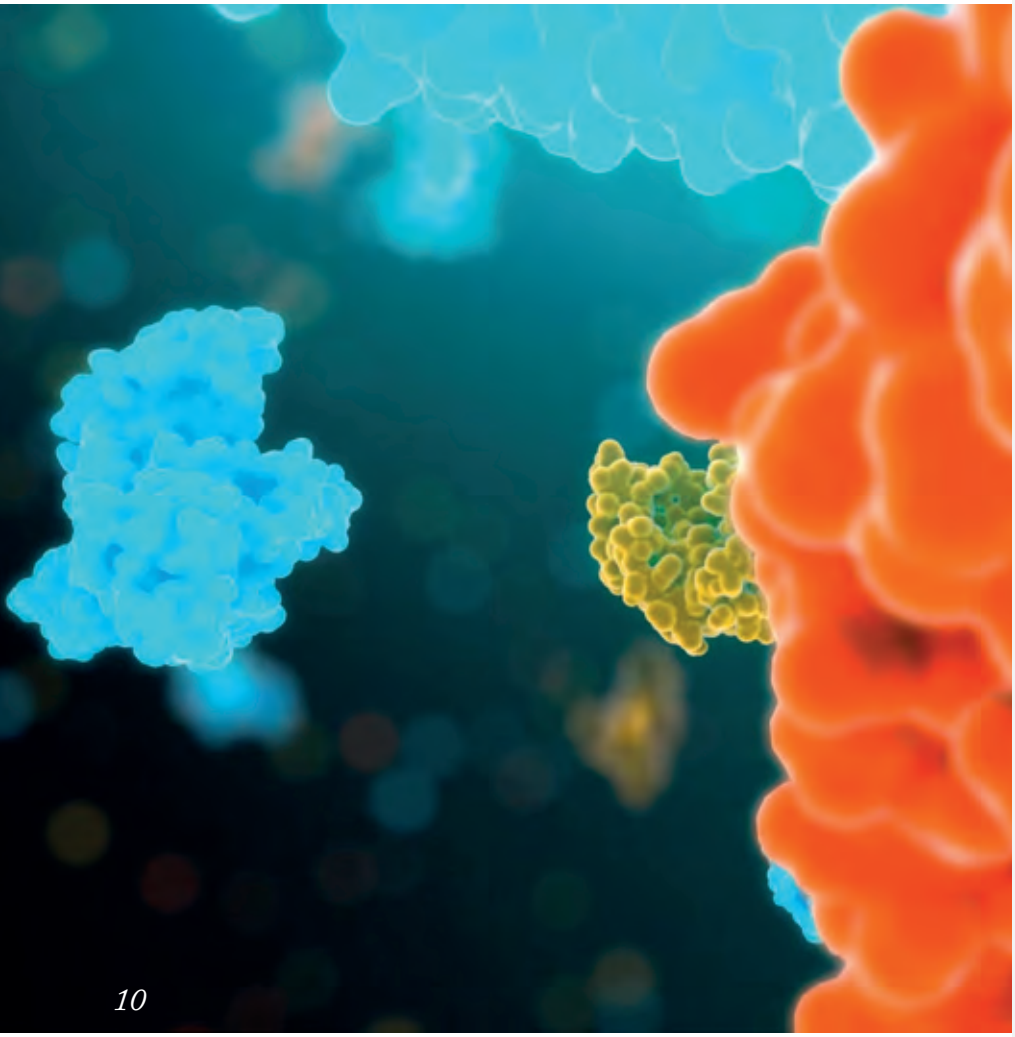

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On The Cover

Women get vocal about (in)equality. Pastiche of Franz Ferdinand's album "You Could Have It So Much Better" (itself a pastiche of Rodchenko's iconic constructivist poster).

Upfront

the Analytical Scientist

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systems can run 24/7 without human intervention, such 'smart' automated systems can facilitate high sample throughput, allowing scientists to focus on the skilled analysis and interpretation of the results rather than on time-consuming wet chemistry or sample injection.

For example, we recently worked on a metabolomics study of algae cell cultures using a PAL RTC platform, which involved a pretty complex pre-analytical process (3). We combined Bligh and Dyer (LLE) extraction with dual-column UHPLC-MS/MS separation and detection in an automated setup (which included adding the set reagents and splitting the aqueous and organic fractions prior to injection into the UHPLC system). Even with an initial manual step, the automated method proved significantly less labor-intensive than the manual technique and also allowed the results to be directly subjected to a library search using LC-MS/MS data in SWATH mode (SCIEX), meaning that further targeted experiments to identify unknowns were unnecessary. Moreover, when compared with the manual method, the automated setup had better repeatability for both aqueous and organic fractions.

Analytical scientists, regardless of industry or sector, are all aiming towards a common goal: achieving the best quality results as efficiently as possible. Taking a smart approach to automating the sample preparation process cuts the 'garbage' being fed into the sample analysis process and improves data quality and speed of delivery to researchers – and thereby reduces the 'garbage' output from the lab.

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On the –Omics Journey

Profiling and fingerprinting in food analysis signposts a route to a better life.

By Chiara Cordero, Associate Professor of Food Chemistry, Department of Drug Science and Technology, University of Turin, Italy.

Modern '-omics' disciplines applied to food (foodomics, sensomics) focus analytical efforts on elucidating bioactive compounds (nutrients and non-nutrients, active secondary metabolites, pre-biotics, odorants and tastants) – essentially, all possible chemical stimuli for food-body interactions (1–3). The ultimate aim is to understand the intriguing – though rather complex – crosstalk between 'what we eat and why, and what we are'. Such investigation requires a comprehensive and integrated approach that will detail a food sample's constituents, in terms of physicochemical properties, concentration in the matrix, distribution throughout the body and, within the "-omics" concept, the physiological activity or sensory properties (odor/taste quality, perception threshold). These comprehensive analyses require multidimensional and hyphenated

analytical platforms capable of exploring all the chemical information dimensions with a detailed profiling approach (4, 5) and all the inter-connecting sample information dimensions (for example, those related to the biological phenomenon being studied) using advanced fingerprinting techniques (6, 7).

'What we eat' is one side of the coin that we need to understand in (chemical) detail so that we know the exact composition to i) differentiate high quality from mass produced products, ii) enable the authentication of a specific botanical/geographical origin or iii) assist technologists during industrial processing with a view to defining a quality benchmark. 'What we are' relates mainly to the interaction of food components within our body. It goes beyond the nutrition domain and includes the effect of non-nutrients and bioactive compounds that may promote health and wellness (nutraceuticals).

Over the last ten years, our research group has dedicated a lot of effort to exploring these concepts and implementing "simple" comprehensive two-dimensional gas chromatographic (GC×GC) platforms and further orthogonal dimensions, including mass spectrometry (MS), olfactometry, automated sample preparation and advanced data mining (8–10). The latter hyphenation, which is fundamental when exploring and interpreting complex data, was realized thanks to the collaboration with experts in other fields. Stephen Reichenbach (Computer Science & Engineering Dept., University of Nebraska–Lincoln, USA) has taken on this challenge and has developed intuitive, effective software solutions for 2D data mining.

Thanks to the superior informing power of GC×GC-MS, we have studied complex fractions of volatiles from high-quality hazelnuts, raw and roasted coffee, green and black tea, dried milk, plant extracts and essential oils. Every analytical run provides a deep insight into the chemical complexity of each sample and provides new perspectives in food chemical investigations that, just a decade ago, were inconceivable – or at least not possible without laborious and time-consuming pre-concentration steps. Looking at the food component distribution and interaction with the body, metabolomics is encouraging collaborative and fascinating studies on the effects of diet and physical exercise on Type 2 diabetes in mice models and in humans (11, 12).

The multi-multi dimensional platforms we have experimented with, thanks to the inspiration of our "boss" (Carlo Bicchi) and the creativity of new generations of scientists, have both intrigued industry and initiated further collaboration. The primary objective? To transfer new concepts in chemical measurements to 'real-world' applications. The vision? To see -omics concepts applied to routine analysis. I believe this will enable quality food chemical characterization, by-product valorization, and bioactive compounds profile activity to be controlled and monitored – all of which will have a positive effect on our lives and society. To that end, academic research must take advantage of the support made available by instrument companies to help direct research effectively through prototyping new analytical solutions for QA and QC laboratories. For example, our collaboration with Agilent and SRA Instruments (Italy) enabled us to transfer most of the "-omics" applications developed for thermal modulated GC×GC-MS platforms to the simpler and cost effective differential flow modulated systems (13–16). Those of you at Riva 2016 will have (had) the chance to see me deliver this work in person (tas.txp.to/0516/riva2016). A prototype is now ready to launch and we are all looking forward to where it will take us on our –omics journey!

References

1–15 Available only online: tas.txp.to/0516/Cordero

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Two Words: Food Scanners

H2020 wanted to put food authentication into the hands of the consumer. What impact will the outcome have on our field?

By Yannick Weesepoel, researcher, Authenticity and Nutrients Business Unit, RIKILT Wageningen UR, The Netherlands.

Two years ago (in June 2014) and by mere coincidence, I entered the field of vibrational spectroscopy. I was starting my first 'real' job as a young researcher at RIKILT in Wageningen. My business unit deals with food authenticity and fraud, multivariate statistics, analytical techniques and many different food types. We looked at what we were doing in the lab and reassigned the tasks, and then I found myself leading the near-infrared, mid-infrared, and Raman spectroscopy division. At that point, I hadn't fully appreciated the revolution going on in the